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Contribution of localized molecular orbitals to the proton magnetic screening constant of PX3 molecules

Aminova R., Zuev M., Morozova I.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

1. A calculation of the magnetic screening constants of the protons in the PH3 and P(CH3)3 molecules with the aid of localized molecular orbitals has been carried out for the first time. 2. The contribution to σ from the canonical and localized molecular orbitals coincide with sufficient accuracy. 3. Localized molecular orbitals make it possible to individually evaluate the contribution of the bonds and lone pairs to the magnetic screening constant. © 1980 Plenum Publishing Corporation.

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